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13. ABSTRACT (Maximum 200 words)

Under support from this grant, we performed work on simulation and design for a number of important topics. These included level set modeling of dendritic solidification, regularized Wulff flows, singularities for flow in porous media, evaluation of American options, epitaxial growth and strain, and electrodeposition.

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FINAL TECHNICAL REPORT
Analytic and Numerical Methods
for Epitaxial Growth and Computer Aided Design

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Under support from this grant, we performed work on simulation and design for a number of important topics. These included level set modeling of dendritic solidification, regularized Wulff flows, singularities for flow in porous media, evaluation of American options, epitaxial growth and strain, and electrodeposition. Key results include the following:

In [1], we developed a new reduced order model for epitaxial growth. The the average coverage, the average island size and the average inter-island distance at each layer of the system. The resulting equations are a system of $3n$ ODEs for a epitaxial film of thickness n layers. This system displays good agreement with the oscillations observed in RHEED measurements during MBE growth, including the variations in the envelope of the oscillations. We expect this model to be useful both for basic understanding and as a tool for control methods.

In [2], we presented a level set approach for the modeling of dendritic solidification. These simulations used a new second order accurate symmetric discretization of the Poisson equation. Numerical results indicated that this method can be used successfully on complex interfacial shapes and can simulate many of the physical features of dendritic solidification. We applied this algorithm to the simulation of the dendritic crystallization of a pure melt and find that the dendrite tip velocity and tip shapes are in excellent agreement with solvability theory. Numerical results were presented in both two and three spatial dimensions.

In [3], we proposed a method of regularizing the backwards parabolic partial differential equations that arise from using gradient descent to minimize surface energy integrals within a level set framework in 2 and 3 dimensions. The proposed regularization energy is a functional of the mean curvature of the surface. Our method used a local level set technique to evolve the resulting fourth order PDEs in time. Numerical results are shown, indicating for the first time, stability and convergence to the asymptotic Wulff shape.

In [4], we analyze the Muskat problem that describes the motion of two fluids of different viscosities in a porous material. This problem is linearly stable if the less viscous fluid is moving into the more viscous fluid and linearly unstable in the reverse case. We find that the linearly unstable problem is ill-posed and can develop singularities on the interface between the two fluids. In addition for linearly stable configuration, we show that there is global existence for initial

data that is sufficiently regular.

In [5, 8, 9], we developed an accelerated numerical method for evaluation of American options. This method is based on the Least Squares Method (LSM) of Longstaff and Schwartz, which used Monte Carlo simulation of the price of the underlying security, combined with a least square regression to perform the projected values that are required in making early exercise decisions. The new feature of our method is the use of quasi-Monte Carlo (QMC) in this problem. Because of the correlation between paths introduced through the regression, it was not obvious that QMC would work on these problems. By using the Brownian bridge construction, we were able to achieve significant acceleration through the use of QMC. This formed part of the PhD thesis of Suneal Chaudhary.

In [10], analyzed a discrete model for atomistic strain in an epitaxial system. The source of strain is the lattice mismatch that occurs in heteroepitaxial growth. For example in growth of Germanium on Silicon. The resulting strain energy can lead to morphological features such as quantum dots. We presented an analysis of the boundary conditions for a strained thin film, and showed that they differ from those of continuum elasticity near a step edge. We also verified the Marchenko-Parshin formula for the stress dipole at a step. This work, as well as our work on level set modeling for epitaxial growth, is reviewed in [11].

In [12], we solved the direct and inverse problems for an electrodeposition developed by Jack Judy (EE Dept, UCLA). His process starts with a series of initially powered and unpowered metallized segments. As the powered segments grow, they may touch an unpowered segment, which will then become powered. In this way they can grow fairly detailed shapes, such as needles, as the micron scale. Our forward solver uses a level set method. Our inverse method is based on a geometric formulation of the model with a power-on time for each point on the electrodeposition surface. Using this we classify the set of achievable geometries, and for any achievable geometry, we find a set of powered and unpowered segments that will lead to an approximation of the desired shape. This formed part of the PhD thesis of Pradeep Thiyanaratnam.

Personnel Supported by this Grant

Russel Caflisch
Stanley Osher
Suneal Chaudhary (graduate student, advised by Caflisch)
Pradeep Thiyanaratnam (graduate student, advised by Caflisch)

Honors and Awards

Russel Caflisch

- Invited speaker. International Congress of Mathematicians, August 2006, Madrid.

Stanley Osher

- Member of the National Academy of Sciences (2005)
- Japan Society of Mechanical Engineering and Computer Mechanics Award (2003)
- ICIAM Pioneer Prize (SIAM 2003)
- Kleinman Prize (SIAM 2005)

Suneal Chaudhary

- PhD. June 2004.

Pradeep Thiyanaratnam

- PhD. June 2006.

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